Computational workflows for the acceleration of ab initio condensed matter theory with machine-learning models.

Contract duration: up to 4 years (2 years renewable once).

Salary: about 30'000€/year gross

Location: IMPMC lab, situated in the Jussieu campus in Paris city center.

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Requisites

A PhD in theoretical condensed matter physics or chemistry, or in computer science. A candidate without PhD, with a degree in Engineering and experience in python development could also be considered.

Context

Financed by National Agency for Research, the PEPR DIADEM is a priority research project financed to develop integrated tools for accelerating the discovery and deployment of emerging new materials. The PEPR is composed of two phases: setting up platforms that provide specific services, then opening external calls for projects that will benefit from said platforms.

The IMPMC institute participates in this effort, in collaboration with the Grenoble University and CEA, by establishing a platform for the ab initio simulation of materials. It comprises standard DFT techniques, advanced methods (QMC, RPA, etc.) to build a database of molecular dynamics trajectory and training sets for machine-learning atomistic potentials.

The researcher will be part of a group of researchers and engineers, working on the combined development of ab initio theory and machine learning methods.The line of work will include both development and applications. The development will involve codes such as Quantum ESPRESSO, VASP, TurboRVB, CP2K, CPMD, Plumed, MetalWalls. Applications will be chosen for their scientific value, but also as challenging samples to foster the platform development.

Tasks

Ensure the reproducibility of numerical simulations, by standardization and containerization of codes. Especially for their use on the French supercomputing centers.

Analysis of sample applications, of scientific and industrial interest, and development of workflows (for example as part of the AiiDA project), with the prospect of reusing them for the projects submitted to the PEPR.

Starting from the second year: consulting, assistance and collaboration in the research of the DIAMOND platform users. Which could comprise scientists with a solid state theory background, experimentalists, engineers.

Collaborate with the Grenoble University on an automated computing center to develop a database of molecular dynamics trajectories.

Skills

- Advanced python programming.
- Basic Fortran and c.
- Knowledge of batch queue systems and experience with computing centers.
- Background in solid state physics.
- Knowledge of docking and container technologies and software environment managers (conda, spack).
- Communication skills.
- English language.